A DFT Study of Glycine Amide Hydrolisis with Water and OH Radical

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The only indisputable evidence on the occurrence of amino acids outside our planet is their detection in carbonaceous chondrites. However only a small fraction was found in a chemically free state, whereas hydrolyzable derivatives of unknown composition (possibly amides) is a major source of the detectable amino acids. The difference between carbonaceous chondrites and the icy bodies (interstellar ices and comets) is the basic component, which is water in the latter case. Thus, it is reasonable to expect a higher content of hydrolized derivatives (free amino acids as final products) in the icy bodies, as compared to that in carbonaceous chondrites. As a preliminary test for energetic feasibility of this type of reaction, we studied theoretically the reaction of glycine amide hydrolysis, at the B3LYP/6-31G++(d,p) level. We found that a very high activation barrier makes this reaction prohibited. Besides molecular water, a similar hydrolytic effect might be produced by hydroxyl radicals (OH) generated under the ionizing action of cosmic rays. Therefore we tested the reaction of glycine amide with OH radical as well. Nevertheless, although the barrier height decreased significantly, by ca. 30 kcal/mol, it remained positive.